L Number	Hits	Search Text	DB	Time stamp
1	697	544/71, 544/101, 514/230.2	USPAT	2004/10/27 13:58
2	80834	microbial or microb\$	USPAT	2004/10/27 13:58
3	70	(544/71, 544/101, 514/230.2) and	USPAT	2004/10/27 13:58
		(microbial or microb\$)		

th

Day: Wednesday

Date: 10/27/2004

Time: 13:59:14

PALM INTRANET

Inventor Information for 10/677551

Inventor Name	City	State/Country
BARBACHYN, MICHAEL ROBERT	ANN ARBOR	MICHIGAN
RUBLE, J. CRAIG	GREENWOOD	INDIANA
ROMERO, ARTHUR GLENN	CHESTERFIELD	MISSOURI
THOMASCO, LISA MARIE	GROTON	CONNECTICUT
HURD, ALEXANDER ROSS	ANN ARBOR	MICHIGAN
PALMER, JOHN RAYMOND	FISHERS	INDIANA
TOOGOOD, PETER LAURENCE	ANN ARBOR	MICHIGAN
MCNAMARA, DENNIS JOSEPH	ANN ARBOR	MICHIGAN
SHERRY, DEBRA ANN	CHELSEA	MICHIGAN
DOBROWOLSKI, PAUL JOSEPH	SALINE	MICHIGAN

Appln Info Contents Petition Info Atty/Agent I	nfo Continuity Data Foreign Data
Search Another: Application#	or Patent# Search
PCT / Search	or PG PUBS #
Attorney Docket #	Search
Bar Code #	arch

To go back use Back button on your browser toolbar.

Back to PALM | ASSIGNMENT | OASIS | Home page



FULL ESTIMATED COST

ENTRY SESSION 0.21 0.21

FILE 'REGISTRY' ENTERED AT 11:52:16 ON 27 OCT 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2004 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 26 OCT 2004 HIGHEST RN 769912-90-5 DICTIONARY FILE UPDATES: 26 OCT 2004 HIGHEST RN 769912-90-5

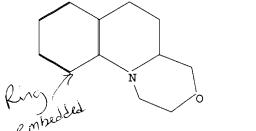
TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

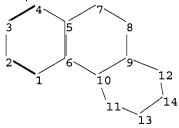
Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at: http://www.cas.org/ONLINE/DBSS/registryss.html

=> Uploading C:\Program Files\Stnexp\Queries\10677551ab.str





ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10 9-12 10-11 11-13 12-14 13-14

exact/norm bonds :

5-7 6-10 7-8 8-9 9-10 9-12 10-11 11-13 12-14 13-14

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:Atom 14:Atom

L1 STRUCTURE UPLOADED

=> s l1

SAMPLE SEARCH INITIATED 11:52:32 FILE 'REGISTRY'

Habte

10/27/2004

10/677,551 Page 3

SAMPLE SCREEN SEARCH COMPLETED -882 TO ITERATE

7 ANSWERS 100.0% PROCESSED 882 ITERATIONS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 15859 TO 19421

7 TO PROJECTED ANSWERS: 298

7 SEA SSS SAM L1 L2

=> s l1 sss full FULL SEARCH INITIATED 11:52:50 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 16937 TO ITERATE

100.0% PROCESSED 16937 ITERATIONS 158 ANSWERS

SEARCH TIME: 00.00.01

L3 158 SEA SSS FUL L1

=> file caplus

COST IN U.S. DOLLARS SINCE FILE TOTAL

SESSION ENTRY 155.42 155.63

FULL ESTIMATED COST

FILE 'CAPLUS' ENTERED AT 11:52:56 ON 27 OCT 2004 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2004 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications. The CA Lexicon is the copyrighted intellectual property of the American Chemical Society and is provided to assist you in searching databases on STN. Any dissemination, distribution, copying, or storing of this information, without the prior written consent of CAS, is strictly prohibited.

FILE COVERS 1907 - 27 Oct 2004 VOL 141 ISS 18 FILE LAST UPDATED: 26 Oct 2004 (20041026/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 13

11 L3 L4

=> d ibib abs hitstr tot

10/27/2004 Habte

ANSWER 1 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN SSION NUMBER: 2004:778888 CAPLUS HENT NUMBER: 141:278615 ACCESSION NUMBER: DOCUMENT NUMBER: TITLE; Photochromic chromenes showing rapid decoloration, and optical materials containing them Izumi, Shinobu: Yamamoto, Hiromasa Tokuyama Corp., Japan Jpn. Kokai Tokkyo Koho, 26 pp. CODEN: JKXXAF INVENTOR(S): PATENT ASSIGNEE(S): SOURCE: DOCUMENT TYPE: Patent Japanese 1 LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

APPLICATION NO. PATENT NO. KIND DATE DATE 20040924 JP 2003-54827 JP 2003-54827 A2 JP 2004262837 20030228 PRIORITY APPLN. INFO.: 20030228

GΙ

Photochromic optical materials (e.g., lenses) contain chromenes I [W = (un)substituted (cyclo)alkylene, (un)substituted arylene: Ri = H, alkyl, aralkyl; Rl may form ring with W: R2, R3 = OH, alkyl, alkoxy, aralkyl, aralkoxy, amino, cyano, NO2, etc.: R4, R5 = alkyl, (un)substituted aryl, aromatic heterocyclyl: R4R5 may form ring: m, n = 0-4]. Thus, aerhylene

polymer material showing Amax 592 nm, coloration d. [ϵ (120) - ϵ (0)] 0.88, decoloration rate (t1/2) 22 s, and inital yellowness index 4.

IT 788691-63-3P

RL: IMF (Industrial manufacture); MOA (Modifier or additive use); PRP (Properties); TEM (Technical or engineered material use); PREP

work

L4 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2004:308443 CAPLUS
DOCUMENT NUMBER: 140:339202
TITLE: Preparation of tricyclic tetrahydroquinoline antibacterial agents
INVENTOR(S): Barbachyn, Michel Robert; Dobrowolski, Faul Joseph; Hurd, Alexander Ross; McNamara, Dennis Joseph; John Raymond; Romero, Arthur Glenn; Ruble, James Craig; Sherry, Debra Ann; Thomasco, Lisa Marie; Toogood, Peter Laurence
Pharmacia & Upjohn Company, USA
PCT Int. Appl., 128 pp.
CODEN: PIXXD2
Patent Palmer,

PATENT ASSIGNEE(S): SOURCE:

DOCUMENT TYPE: Patent English 1 FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

	PATENT NO.																	
WC										WO 2003-IB4389								
	W:						AU,											
		co,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	EG,	ES,	FΙ,	GB,	GD,	GE,	
		GH,	GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,	ΚP,	KR,	ΚZ,	LC,	LK,	
		LR,	LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NI,	NO,	NZ,	
		OM,	PG,	PH,	PL,	PT,	RO,	RU,	SC,	SD,	SE,	SG,	SK,	SL,	SY,	ТJ,	TM,	
		TN,	TR,	TT,	TZ,	UA,	UG,	US,	UZ,	VC,	VN,	YU,	ZA,	ZM,	ZW,	AM,	AZ,	
		BY,	KG,	KZ,	MD													
	RW:	GH,	GM,	KE,	LS,	MW,	MZ,	SD,	SL,	SZ,	TZ,	UĢ,	ZM,	ZW,	ΑT,	BE,	BG,	
		CH,	CY,	CZ,	DE,	DK,	EE,	ES,	FI,	FR,	GB,	GR,	HU,	IE,	IT,	LU,	MC,	
		NL,	PT,	RO,	SE,	SI,	sĸ,	TR,	BF,	ВJ,	CF,	CG,	CI,	CM,	GΑ,	GN,	GQ,	
							TD,											
	2004																	
RIORIT	ORITY APPLN. INFO.:								US 2	002-	4166	85P		P 2	0021	007		
										US 2	002-	4271	89P		P 2	0021	118	
										US 2	003-	4576	22P		P 2	0030	326	

MARPAT 140:339202 OTHER SOURCE(S):

$$(\mathbb{R}^4)_{1?3} \xrightarrow{\mathbb{R}^3}_{\mathbb{R}^5} \mathbb{R}^1$$

$$\mathbb{R}^4$$

$$\mathbb{R}^4$$

$$\mathbb{R}^5$$

AB The invention includes tricyclic tetrahydroquinolines (shown as I;

Habte

PF

ANSWER 1 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN (Preparation); USES (Uses) (manuf. of photochromic chromenes for lenses) 758691-63-3 CAPLUS INDEX NAME NOT YET ASSIGNED (Continued)

IT RE: RCT (Reactant); RACT (Reactant or reagent)
[manufacture of photochromic chromenes for lenses)
758691-72-4 CAPLUS
INDEX NAME NOT YET ASSIGNED

ANSWER 2 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN (Continued) variables defined below; many of the examples are spiro compds., e.g.

variables defined below; many of the examples are spiro compds., e.g. and trans-II), and pharmaceutical compns. thereof, that exhibit useful antibacterial activity against a wide range of human and veterinary pathogens. For I: Rl is R12, C(O)R6, or CN: R2 = R12, C(O)R7, CN, CK2R7, NR17R7, CH2COR7, CH2CH2COR7, R3 = H, R2, O, C1-7 alkyl, C3-8 eycloalkyl, aryl, heteroaryl, or halo: each R4 = H, halo, OR12, OC(O)NR9R10, SR12, S(O)mR13, NR9R10, NR9C(O)mR13, R12, Ph, heteroaryl, eyano, nitro, CONR9R10, CO2R12, C(O)R13, C(:NOR12)R13, S(O)mNR9R10, NR9C(O)R12, C1-7 alkyl, C3-8 cycloalkyl, N3, hetl, or C(O)O-C1-4alkyl-R12 each R5 = H, C1-7alkyl, C3-8cycloalkyl, aryl or heteroaryl: X = -(C(R15)2)H--, -[C(R15)2]K-, -[C(R15)2]K-, -[C(R15)2]K-, -[C(R15)2]K-, or heteroaryl: Hetl is a C- or N-linked 5-8 membered mono- or bicyclic ring, each mono- or bicyclic ring being fully sato. or partially unsatd., and having 1-4 heteroatoms O, S, and N; hetl being (un)substituted by 1-2 substituents = C1-dalkyl, amino, C1-C4alkylamino, C1-C4alkyloxy, gen.

halogen,
CN, O, or S; addnl. details including provisos are given in the claims.

method of prepn. is claimed and .apprx.60 example prepns. are included. For example, cis- and trans-II were prepd. in 3 steps starting with condensation of 2-fluoro-5-nitrobenzaldehyde with 2,6-dimethylmorpholine to give cis- and trans-2-[2-(2-6-dimethylmorpholin-4-yl)-5-nitrobenzaldehyde, each of which was condensed with barbituric acid to give cis- and trans-5-[2-(2-6-dimethylmorpholin-4-yl)-5-nitrobenzylidene|pyrimidine-2,4,6(1M,3M,5M)-trione, resp., each of which was cyclized in refluxing MeOH. Inhibition of E. coli DNA gyrase by 12 examples of I are reported. IT 679839-05-5F
RL: PAC (Pharmacological activity); PEP (Physical, engineering or chemical

ical
process); PYP (Physical process); RCT (Reactant); SPN (Synthetic
preparation); THU (Therapeutic use); EJOL (Biological study); PREP
(Preparation); PROC (Process); RACT (Reactant or reagent); USES (Uses)
(drug candidate, chromatog, resolution; preparation of tricyclic
tetrahydroquinoline antibacterial agents)
679839-05-5 CAPLUS
Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine] 2',4',6'(1'H,3'H)-trione, 1,2,4,4a-tetrahydro-2,4-dimethyl-8-nitro-,
(2R,4S)-rel- (SCI) (CA INDEX NAME)

L4 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

IT 679839-36-2P 679839-41-9P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREF (Preparation); RRCT (Reactant or reagent); USES (Uses) (drug candidate; preparation of tricyclic tetrahydroquinoline antibacterial agents)
RN 679839-36-2 CAPLUS
CN Carbamic acid, [{2R,4S,4aS}-1,1',2,3',4,4',4a,6'-octahydro-2,4-dimethyl-

2',4',6'-trioxospiro[[1,4]oxazino[4,3-a]quinoline-5[6H),5'(2'H)-pyrimidin]-8-yl]-, 1,1-dimethylethyl ester, rel- (9CI) (CA INDEX NAME)

679839-41-9 CAPLUS Spiro[[1,4]oxazino[4,3-a]quinoline-5[6H],5'(2'H)-pyrimidine]-2',4',6'(1'H,3'H)-trione, 8-acetyl-1,2,4,4a-tetrahydro-2,4-dimethyl-, (2R,4S,4a5)-rel- [9CI] (CA INDEX NAME)

ANSWER 2 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN (Continued) 679840-95-09 681006-33-79
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES

(Uses) (drug candidate; prepn. of tricyclic tetrahydroquinoline antibacterial agents) (drug candidate; prepn. of tricyclic tetrahydroquinoline antibacterial agents) (679839-06-6 CAPLUS Spiro([1,4]) (2798-2008)

Relative stereochemistry.

679839-11-3 CAPLUS
Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]2',4',6'[1'H,3'H)-trione, 1,2,4,4a-tetrahydro-2,4-dimethyl-,
(2R,4S,4aS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

679839-13-5 CAPLUS
Spiro[[1,4]0xazino[4,3-a]quinoline-5[6H),5'[2'H]-pyrimidine]2',4',6'[1'H,3'H]-ttione, 8-bromo-1,2,4,4a-tetrahydro-2,4-dimethyl-,
(2R,4S,4aS)-rel- (9CI) (CA INDEX NAME)

L4 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN (Continued) Relative stereochemistry.

679839-06-6F 679839-11-3F 679839-13-5F 679839-16-8F 679839-12-6F 679839-12-6F 679839-13-17F 679839-22-6F 679839-26-0F 679839-26-0F 679839-26-0F 679839-34-0F 679839-31-7F 679839-33-79 679839-34-0F 679839-31-7F 679839-33-73-7F 679839-34-6-6F 679839-55-0F 679839-55-2F 679839-55-5F 679839-55-5F 679839-55-5F 679839-55-5F 679839-55-5F 679839-55-5F 679839-55-5F 679839-55-5F 679839-56-6F 679839-61-6F 679840-61-9F 679840-31-6F 679840-31-6F

ANSWER 2 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

679839-16-8 CAPLUS
Spiro[[1,4]oxazino[4,3-a]quinoline-5[6H],5'[2'H]-pyrimidine]2',4',6'[1'H,3'H]-trione, 8-fluoro-1,2,4,4a-tetrahydro-2,4-dimethyl-,
(2R,4S,4aS)-rel- [9CI] (CA INDEX NAME)

Relative stereochemistry.

679839-19-1 CAPLUS Spirof(1,4)oxazino(4,3-a)quinoline-5(6H),5' $(2^{\dagger}H)$ -pyrimidine}-2',4',6' $(1^{\dagger}H)$ 3'H)-trione, 1,2,4,4a-tetrahydro-2,4-dimethyl-8-(trifluoromethyl)-, (2R,45,4aS)-rel-(9CI) (CA INDEX NAME)

L4 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

RN 679839-22-6 CAPLUS CN spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]-8-carbonitrile, 1,1',2,3',4,4',4,6'-octahydro-2,4-dimethyl-2',4',6'-trioxo-, (2R,4S,4aS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 679839-24-8 CAPLUS
Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]-8carboxanide,
1,1',2,3',4,4',4a,6'-octahydro-2,4-dimethyl-2',4',6'-trioxo-,
(2R,483)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

ANSWER 2 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

RN 679839-33-9 CAPLUS
CN Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]4',6'[1'H,3'H]-dione,
8-bromo-1,2,4,4a-tetahydro-2,4-dimethyl-2'-thioxo-,
(2R,4S,4aS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

679839-34-0 CAPLUS Spiro[[1,4]0xazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]-2',4',6'(1'H,3'H)-trione, B-bromo-1,2,4,4a-tetrahydro-1',2,3',4-tetramethyl-, (2R,4S,4a5)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

L4 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

679839-26-0 CAPLUS Spiro([1,4]oxazino[4,3-a]quinoline-5(6H),5'{2'H}-pyrimidine]-2',4',6'(1'H,3'H)-trione, 1,2,4,4a-tetrahydro-8-nitro- (9CI) (CA INDEX NAME)

679839-27-1 CAPLUS Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]-2',4',6'(1'H,3'H)-trione, 1,2,4,4a-tetrahydro- (9CI) (CA INDEX NAME)

679839-31-7 CAPLUS Spire{[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]-2',4',6'(1'H,3'H)-trione, 1,2,4,4a-tetrahydro-1,4a-dimethyl-8-nitro-(9CI)

L4 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

679839-35-1 CAPLUS Acetamide, N-[(2R,4S,4aS)-1,1',2,3',4,4',4a,6'-octahydro-2,4-dimethyl-

2',4',6'-trioxospiro([1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidin]-8-yl]-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

679839-37-3 CAPLUS
Spirof([1,4]0xazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]2',4',6'(1'H,3'H)-trione, 8-amino-1,2,4,4a-tetrahydro-2,4-dimethyl-,
monohydrochloride, {2R,4S,4aS}-rel- (9CI) {CA INDEX NAME}

L4 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN (Continue

• HCl

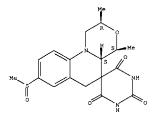
RN 679839-38-4 CAPLUS
CN Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]2',4',6'(1'H,3'H)-trione,
9-bromo-1,2,4,4a-tetrahydro-2,4-dimethyl-8-nitro, (2R,4S,4aS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 679839-44-2 CAPLUS
Spiro[[1,4]0xazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]2',4',6'(1'H,3'H)-trione, 1,2,4,4a-tetrahydro-8-[1-(methoxyimino)ethyl]2,4-dimethyl-, (2R,4S,4aS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry unknown.

L4 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



RN 679839-50-0 CAPLUS
CN Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]2',4',6'(2'H,3'H)-trione,
1,2,4,4a-tetrahydro-2,4-dimethyl-8-(methylthio), (2R,4S,4aS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 679839-52-2 CAPLUS
Spirof[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]2',4',6'(1'H,3'H)-trione, 1,2,4,4a-tetrahydro-2,4-dimethyl-9-nitro-,
[2R,4S,4aS]-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

L4 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

RN 679839-45-3 CAPLUS
CN Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]2',4',6'(1'H,3'H)-trione, 1,2,4,4a-tetrahydro-2,4-dimethyl-8(methylsulfonyl)-, (2R,48,4as)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 679839-48-6 CAPLUS
CN Spiro[[1,4]0xazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]2',4',6'(1'H,3'H)-trione, 1,2,4,4a-tetrahydro-2,4-dimethyl-8(methylsulfinyl)-, (2R,4S,4aS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

L4 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

RN 679839-55-5 CAPLUS
Spiro[[1,4]oxazino[4,3-a]quinoline=5(6H),5'(2'H)-pyrimidine]2',4',6'('H,3'H)-trione, 1,2,4,4a-tetrahydro-1',2,3',4-tetramethyl-8nitro-, (2R,48,4as)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 679839-56-6 CAPLUS
CN Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]2',4',6'(2'H,3'H)-trione, 1,2,4,4a-tetrahydro-1',2,4-trimethyl-8-nitro-,
{2R,4S,4aS}-rel- {9CI} (CA INDEX NAME)

L4 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

679839-57-7 CAPLUS spiro([1,4]oxarino(4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]2',4',6'(1'H,3'H)-trione, 1,2,4,4a-tetrahydro-4-methyl-8-nitro- (9CI)

679839-58-8 CAPLUS Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]-2',4',6'(1'H,3'H)-trione, 1,2,4,4a-tetrahydro-2-methyl-8-nitro- (9CI)

INDEX NAME)

L4 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN

679839-68-0 CAPLUS
Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]2',4',6'(1"H,3'H)-trione, 9-(4-chlorophenyl)-1,2,4,4a-tetrahydro-2,4dimethyl-, (2R,48,4a8)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

679839-71-5 CAPLUS
Spiro([1,4]oxazino(4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]2',4',6'(1'H,3'H)-trione, 1,2,4,4a-tetrahydro-2,4-dimethyl-9-[4(trifluoromethoxy)phenyl]-, (2R,4S,4aS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

ANSWER 2 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN (Continued) 679839-63-5 CAPLUS Spiro(2H-indene-2,5'(6'H)-{1,4}cvazino[4,3-a]quinoline]-8'-carbonitrile, 1,1',2',3,4',4'a-hexahydro-2',4'-dimethyl-1,3-dioxo-, (2'R,4'S,4'aR)-rel-(9CI) (CA INDEX NAME)

Relative stereochemistry.

679839-64-6 CAPLUS
[1,4]Oxazino[4,3-a]quinoline-5,5,8(6H)-tricarbonitrile,
1,2,4,4a-tetrahydro-2,4-dimethyl-, (2R,4s,4aR)-rel- (9CI) (CA INDEX

Relative stereochemistry.

679839-65-7 CAPLUS
[1,4]Oxazino[4,3-a]quinoline-5,5(6H)-dicarbonitrile, 8-bromo-1,2,4,4a-tetrahydro-2,4-dimethyl-, (2R,4S,4aR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

L4 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN

(Continued)

679839-73-7 CAPLUS Spiro([1,4]0xazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]-2',4',6'(1'H,3'H)-trione, 1,2,4,4a-tetrahydro-9-(4-methoxypheny1)-2,4-dimethyl-, (2R,4S,4aS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 679839-74-8 CAPLUS
CN Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine)2',4',6'(1'H,3'H)-trione,
9-(3-chloro-4-fluorophenyl)-1,2,4,4a-tetrahydro2,4-dimethyl-, (2R,45,4as)-rel- (9CI) (CA INDEX NAME)

L4 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

679839-76-0 CAPLUS Spirof[[1,4]0xazino[4,3-a]quinoline-5[6H],5'[2'H]-pyrimidine]-2',4',6'[1'H,3'H]-trione, 1,2,4,4a-tetrahydro-2,4-dimethyl-9-(3-nitrophenyl)-, (2R,4S,4aS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

679839-78-2 CAPLUS Benzonitrile, 4-[(2R,4S,4aS)-1,1',2,3',4,4',4a,6'-octahydro-2,4-dimethyl-

2',4',6'-trioxospiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidin]-9-yl]-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

ANSWER 2 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

679839-83-9 cRPLUS
Spiro[[1,4]oxazino[4,3-a]quinoline-5[6H],5'(2'H)-pyrimidine]-9-carboxylic
acid, 1,1',2,3',4,4',4a,6'-octahydro-2,4-dimethyl-2',4',6'-trioxo-,

ester, (2R,4S,4aS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

679839-84-0 CAPLUS
Spiro[(1,4]oxazino(4,3-a]quinoline-5(6H),5'{2'H}-pyrimidine]-8-carboxylic
acid, 1,1',2,3',4,4',4a,6'-octahydro-2,4-dimethyl-2',4',6'-trioxo-, 679839-84-0 CAPLUS

methyl ester, (2R,4S,4aS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

L4 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

679839-80-6 CAPLUS Spiro([1,4]0xazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]-2',4',6'(1'H,3'H)-trione, 1,2,4,4a-tetrahydro-2,4-dimethyl-9-[4-(methylsulfonyl)phenyl]-, (2R,4S,4aS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 679839-82-8 CAPLUS
CN Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]2',4',6'(1'H,3'H)-trione,
1,2,4,4-tetrahydro-2,4-dimethyl-9-(4-pyridinyl), (2R,4S,4aS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

L4 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN

679839-87-3 CAPLUS
Spiro[[1,4]0xazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]2',4',6'(1'H,3'H)-trione, 2,4-diethyl-1,2,4,4a-tetrahydro-8-nitro-,
(2R,4S,4as)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

679839-92-0 CAPLUS
Spiro([1,4]oxazino(4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]2',4',6'(1'H,3'H)-trione, 1,2,4,4a-tetrahydro-4-methyl-8-nitro-2(trifluoromethyl)-, (2R,4R,4aR)-rel- (9CI) (CA INDEX NAME)

L4 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

RN 679839-99-7 CAPLUS
Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]2',4',6'('H,3'H)-trione, 1,2,4,4a-tetrahydro-4-methyl-8-nitro-2-propyl-,
(2R,4S,4aS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 679840-05-2 CAPLUS
Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]2',4',6'(1'H,3'H)-trione, 1,2,4,4a-tetrahydro-2,4-dimethyl-8-nitro-,
(25,4s,4a5)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

RN 679840-19-8 CAPLUS
Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine}2',4',6'(1'H,3'H)-trione, 10-fluoro-1,2,4,4a-tetrahydro-2,4-dimethyl-8nitro-, (2R,4S,4aS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 679840-23-4 CAPLUS
Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]2',4',6'(1'H,3'H)-trione, 1,2,4,4a-tetrahydro-2,4-dimethyl-8-(5-methyl-1,2,4-oxadlazol-3-yl)-, (2R,4S,4aS)-rel-[9CI] (CA INDEX NAME)

Relative stereochemistry.

L4 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

RN 679840-13-2 CAPLUS
Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]2',4',6'('H,3'H)-trione, 8-acetyl-10-fluoro-1,2,4,4a-tetrahydro-2,4dimethyl-, (2R,4S,4aS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry

RN 679840-15-4 CAPLUS
Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]2',4',6'(1'H,3'H)-trione, 8-acetyl-9,10-diffluoro-1,2,4,4a-tetrahydro-2,4dimethyl-, (2R,4S,4aS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

L4 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

RN 679840-25-6 CAPLUS
Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]2',4',6'('H,3'H)-trione, 1,2,4,4a-tetrahydro-2,4-dimethyl-8-{3-methyl-1,2,4-oxadiazol-5-yl)-, {2R,48,4as}-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 679840-29-0 CAPLUS
Spiro{[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]-8carboxaldehyde, 1,1',2,3',4,4',4a,6'-octahydro-2,4-dimethyl-2',4',6'trioxo-, (2R,4S,4aS)-rel- (9CI) (CA INDEX NAME)

L4 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

RN 679840-31-4 CAPLUS
Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]2',4',6'(1'H,3'H)-trione, 1,2,4,4a-tetrahydro-2,4-dimethyl-8-nitro-,
(2R,4S,4aS)-rel-(-)- (9CI) (CA INDEX NAME)

Rotation (-). Absolute stereochemistry unknown.

RN 679840-32-5 CAPLUS Spiro[[1,4]0xazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]-2',4',6'(1'H,3'H)-trione, 1,2,4,4a-tetrahydro-2,4-dimethyl- (9CI) (CA INDEX NAME)

L4 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN (Continued) 2',4',6'(1'H,3'H)-trione, 1,2,4,4a-tetrahydro-2,4-dimethyl-8-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 679840-36-9 CAPLUS
CN Spiro[{1,4]cazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]-8carbonitrile,
1,1',2,3',4,4',4,6'-octahydro-2,4-dimethyl-2',4',6'-trioxo(9C1) (CA INDEX NAME)

RN 679840-37-0 CAPLUS
Spirc([1,4)oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]-8carboxamide, 1,1',2,3',4,4',4a,6'-octahydro-2,4-dimethyl-2',4',6'-trioxo(SCI) (CA INDEX NAME)

RN 679840-38-1 CAPLUS
CN Acetamide, N-(1,1',2,3',4,4',4a,6'-octahydro-2,4-dimethyl-2',4',6'-trioxospiro[[1,4]cxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidin]-8-yl)-

Habte

L4 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

RN 679840-33-6 CAPLUS
CN Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H],5'(2'H)-pyrimidine]2',4',6'(1'H,3'H)-trione, 8-bromo-1,2,4,4a-tetrahydro-2,4-dimethyl- (9CI)
(CA INDEX NAME)

RN 679840-34-7 CAPLUS
Spiro([1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]2',4',6'(1'H,3'H)-trione, 8-fluoro-1,2,4,4a-tetrahydro-2,4-dimethyl(9CI)
(CA INDEX NAME)

RN 679840-35-8 CAPLUS CN Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]-

L4 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN (Continued) (9CI) (CA INDEX NAME)

RN 679840-39-2 CAPLUS
Carbamic acid, (1,1',2,3',4,4',4a,6'-octahydro-2,4-dimethyl-2',4',6'trioxospiro[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidin)-8-yl)-,
1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 679840-40-5 CAPLUS

Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]2',4',6'(1'H,3'H)-trione, 8-amino-1,2,4,4a-tetrahydro-2,4-dimethyl-,
monohydrochloride (9CI) (CA INDEX NAME)

• HCl

RN 679840-41-6 CAPLUS 10/27/2004 L4 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
CN Spiro[[1,4] oxazino[4,3-a] quinoline-5(6H),5'(2'H)-pyrimidine]2',4',6'(1'H,3'H)-trione,
9-bromo-1,2',4,4-at-terahydro-2,4-dimethyl-8-nitro(9CI) (CA INDEX NAME)

Br NH

RN 679840-42-7 CAPLUS
CN Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]2',4',6'(1'H,3'H)-trione, 8-acetyl-1,2,4,4a-tetrahydro-2,4-dimethyl-

(CA INDEX NAME)

Ac O Me O NH

RN 679840-43-8 CAPLUS
CN Spiro[[1,4] oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]2',4',6'(1'H,3'H)-trione, 1,2,4,4a-tetrahydro-8-[1-(methoxyimino)ethyl]2,4-dimethyl- (9CI) (CA INDEX NAME)

L4 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN (Continued) (SCI) (CA INDEX NAME)

RN 679840-47-2 CAPLUS
Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]2',4',6'(1'H,3'H)-trione, 1,2,4,4a-tetrahydro-2,4-dimethyl-9-nitro-(9CI)
(CA INDEX NAME)

RN 679840-48-3 CAPLUS
CN Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]2',4',6'(1'H,3'H)-trione, 1,2,4,4a-tetrahydro-1',2,3',4-tetramethyl-8nitro- (9CI) (CA INDEX NAME)

RN 679840-49-4 CAPLUS
CN Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]2',4',6'(1'H,3'H)-trione, 1,2,4,4a-tetrahydro-1',2,4-trimethyl-8-nitro(9CI) {CA INDEX NAME}

Habte

L4 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

RN 679840-44-9 CAPLUS
CN Spiro[[1,4]oxazlno[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]2',4',6'(1'H,3'H)-trione, 1,2,4,4a-tetrahydro-2,4-dimethyl-8(methylsulfonyl)- (9CI) (CA INDEX NAME)

RN 679840-45-0 CAPLUS
CN Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]2',4',6'(1'H,3'H)-trione, 1,2,4,4a-tetrahydro-2,4-dimethyl-8(methylsulfinyl)- (9CI) (CA INDEX NAME)

RN 679840-46-1 CAPLUS
Spiro{[1,4]oxazino[4,3-a]quinoline-5{6H},5'{2'H}-pyrimidine]2',4',6'[1],3'[H]-trione,
1,2,4,4a-tetrahydro-2,4-dimethyl-8-(methylthio)-

L4 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

RN 679840-50-7 CAPLUS
CN Spiro[2H-indene-2,5'(6'H)-[1,4]oxazino[4,3-a]quinoline]-8'-carbonitrile,
1,1',2',3,4',4'a-hexahydro-2',4'-dimethyl-1,3-dioxo-(9CI) (CA INDEX NAME)

RN 679840-51-8 CAPLUS [1,4]0xazino[4,3-a]quinoline-5,5,8(6H)-tricarbonitrile, 1,2,4,4a-tetrahydro-2,4-dimethyl- (9CI) (CA INDEX NAME)

RN 679840-52-9 CAPLUS
CN [1,4]Oxazino[4,3-a]quinoline-5,5(6H)-dicarbonitrile, 8-bromo-1,2,4,4a-tetrahydro-2,4-dimethyl- (9CI) (CA INDEX NAME)

(Continued) L4 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN

679840-53-0 CAPLUS
Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]2',4',6'(1'H,3'H)-trione, 9-(4-chlorophenyl)-1,2,4,4a-tetrahydro-2,4dimethyl- (9CI) (CA INDEX NAME)

679840-54-1 CAPLUS
Spiro[[1,4]0xazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]2',4',6'(1'H,3'H)-trione, 1,2,4,4a-tetrahydro-2,4-dimethyl-9-[4-(trifluoromethoxy)phenyl]- (9CI) (CA INDEX NAME)

679840-55-2 CAPLUS
Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]2',4',6'(1'H,3'H)-trione, 1,2,4,4a-tetrahydro-9-(4-methoxyphenyl)-2,4-dimethyl- (9CI) (CA INDEX NAME)

ANSWER 2 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN (Continued) trioxospiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'[2'H)-pyrimidin]-9-y1)-(9CI) (CA INDEX NAME)

679840-59-6 CAPLUS
Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]2',4',6'(1'H,3'H)-trione, 1,2',4',4a-tetrahydro-2',4-dimethyl-9-[4-(methylsulfonyl)phenyl}- (9CI) (CA INDEX NAME)

RN 679840-60-9 CAPLUS

CN Spiro[[1,4]0xaZino[4,3-a]quinoline-5[6H),5'(2'H)-pyrimidine]2',4',6'(1'H,3'H)-trione,
1,2,4,4a-tetrahydro-2,4-dimethyl-9-(4-pyridinyl)[9CI] (CA INDEX NAME)

679840-61-0 CAPLUS Spire[[1,4]exazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]-9-carboxylic acid. 1,1',2,3',4,4',4a,6'-octahydro-2,4-dimethyl-2',4',6'-trioxo-,

L4 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN

679840-56-3 CAPLUS
Spiro[[1,4]oxazino[4,3-a]quinoline-5[6H],5'(2'H)-pyrimidine]2',4',6'[1'H,3'H]-trione,
-chloro-4-fluorophenyl]-1,2,4,4a-tetrahydro2,4-dimethyl- [9CI] (CA INDEX NAME)

679840-57-4 CAPLUS Spiro[[1,4]0xazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]-2',4',6'(1'H)-trione, 1,2,4,4a-tetrahydro-2,4-dimethyl-9-(3-nitrophenyl)- (9CI) (CA INDEX NAME)

679840-58-5 CAPLUS Benzonitrile, 4-(1,1',2,3',4,4',4a,6'-octahydro-2,4-dimethyl-2',4',6'-

ANSWER 2 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN ester (9CI) (CA INDEX NAME) (Continued)

679840-62-1 CAPLUS Spiro([1,4]0xazino(4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]-8-carboxylic acid, 1,1',2,3',4,4',4a,6'-octahydro-2,4-dimethyl-2',4',6'-trioxo-, methyl

ester (9CI) (CA INDEX NAME)

679840-63-2 CAPLUS kN 6/9840-63-2 CAPLUS
Spiro([1,4]0xazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]2',4',6'(1'H,3'H)-trione,
1,2,4,4-tetrahydro-2-methyl-4-(1-methylethyl)-8nitro-, (28,4R,4aR)- (9CI) (CA INDEX NAME)

L4 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

RN 679840-64-3 CAPLUS
Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'{2'H}-pyrimidine]2',4',6'{1'H,3'H}-trione, 2,4-diethyl-1,2,4,4a-tetrahydro-8-nitro-,
(2R,4S,4aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 679840-65-4 CAPLUS Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]-2',4',6'(1'H,3'H)-trione, 8-acetyl-9,10-difluoro-1,2,4,4a-tetrahydro-2,4dimethyl-, (2R,4S,4as)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

RN 679840-68-7 CAPLUS
Spiro[[],4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]2',4',6'(1'H,3'H)-trione, 1,2,4,4a-tetrahydro-2,4-dimethyl-8-nitro-(9CI)
(CA INDEX NAME)

RN 679840-69-8 CAPLUS
CN Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]2',4',6'(1'H,3'H)-trione,
1,2',4,4-tetrahydro-4-methyl-2-(1-methylethyl)-8nitro-, (2S,4R,4aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

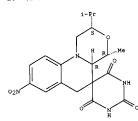
RN 679840-66-5 CAPLUS
Spiro([1,4]0x8zino(4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine)2',4',6'(1'H,3'H)-trione, 10-fluoro-1,2,4,4a-tetrahydro-2,4-dimethyl-8nitro-, (2R,45,4aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 679840-67-6 CAPLUS
Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]2',4',6'(1'H,3'H)-trione, 1,2,4,4a-tetrahydro-2,4-dimethyl-8-[5(trifluoromethyl)-1,2,4-oxadiazol-3-yl]-, (2R,4S,4aS)- (9CI) (CA INDEX NOVEL)

Absolute stereochemistry.

L4 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN (C



RN 679840-70-1 CAPLUS
Spiro([1,4]oxazino[4,3-a]quinoline=5[6H),5'(2'H)-pyrimidine}2',4',6'('1H,3'H)-trione, 1,2,4,4a-tetrahydro-2,4-bis(1-methylethyl)-8nitro-, (2R,45,4as)- (9CI) (CA INDEX NAME)

Absolute stereochemistry

RN 679840-71-2 CAPLUS Spiro[[1,4]oxazino[4,3-a]quinoline-5[6H],5'[2'H]-pyrimidine]-2',4',6''[1'H,3'H]-trione, 1,2,4,4a-tetrahydro-2,4-dimethyl-8-(3-methyl-1,2,4-oxadiazol-5-yl)-, (2R,4S,4aS)- (9CI) (CA INDEX NAME)

L4 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

RN 679840-72-3 CAPLUS
Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]2',4',6'('H,3'H)-trione, 8-acetyl-10-fluoro-1,2,4,4a-tetrahydro-2,4dimethyl-, (2S,4R,4aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 679840-74-5 CAPLUS
Spiro([1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]2',4',6'(1'H,3'H)-trione, 8-bromo-1,2,4,4a-tetrahydro-2,4-dimethyl-10nitro- (9Cl) (CA INDEX NAME)

L4 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN

(Continued)

RN 679840-75-6 CAPLUS
Spirof[11,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]21,4',6'(1H,3'H)-trione, 1,2,4,4a-tetrahydro-2,4-dimethyl-8-(5-methyl1,2,4-oxadiazol-3-yl)-, (2R,4S,4aS)- [9CI] (CA INDEX NAME)

Absolute stereochemistry.

RN 679840-76-7 CAPLUS
Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]2',4',6'(1'H,3'H)-trione, 1,2,4,4a-tetrahydro-4-methyl-8-nitro-2(trifluoromethyl)-, (2S,4S,4aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

RN 679840-77-8 CAPLUS
Spiro[[1,4]0xazino[4,3-a]quinoline-5[6H],5'(2'H)-pyrimidine]-8-carboxylic
acid, 1,1',2,3',4,4',4a,6'-octahydro-2,4-dimethyl-2',4',6'-trioxo-,
(4-azido-3-lodophenyl)methyl ester, (2R,4S,4aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 679840-78-9 CAPLUS
Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]2',4',6'(1'H,3'H)-trione, 1,2,4,4a-tetrahydro-4-methyl-8-nitro-,
(4R,4aR)-rel-(-)- (9CI) (CA INDEX NAME)

Rotation (-). Absolute stereochemistry unknown.

L4 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN

(Continued)

RN 679840-79-0 CAPLUS
CN Spiro[{1,4}oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]4',6'(1'H,3'H)-dione,
8-bromo-1,2,4,4a-tetrahydro-2,4-dimethyl-2'-thioxo-,
{2R,4S,4aS}- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 679840-80-3 CAPLUS Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]-2',4',6'(1'H,3'H)-trione, 8-bromo-1,2,4,4a-tetrahydro-1',2,3',4-tetramethyl-,(2R,4S,4aS)-(9CI) (CA INDEX NAME)

(Continued) L4 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN

679840-81-4 CAPLUS Spiro(2H-indene-2,5'(6'H)-[1,4]oxazino[4,3-a]quinoline]-8'-carbonitrile, 1,1',2',3,4',4'a-hexahydro-2',4'-dimethyl-1,3-dioxo-, (2'R,4'S,4'aS)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

679840-82-5 CAPLUS
[1,4]Oxazino[4,3-a]quinoline-5,5,8[6H]-tricarbonitrile,
1,2,4,4a-tetrahydro-2,4-dimethyl-, (2R,45,4aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN

(Continued)

679840-83-6 CAPLUS [], 4] OMAZINO [4, 3-a] quinoline-5, 5 (6H)-dicarbonitrile, 8-bromo-1, 2, 4, 4a-tetrahydro-2, 4-dimethyl-, (2R, 4S, 4aS) - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

679840-85-8 CAPLUS
Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]2',4',6'(1'H,3'H)-trione, 9-(4-chlorophenyl)-1,2,4,4a-tetrahydro-2,4dimethyl-, (2R,48,4aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 2 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

679840-86-9 CAPLUS
Spiro[[1,4]0xazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]2',4',6'(1'H,3'H)-trione, 1,2,4,4a-tetrahydro-2,4-dimethyl-9-[4-(trifluoromethoxy)phenyl]-, (2R,4S,4aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

679840-88-1 CAPLUS Spiro[[1,4]exazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]-2',4',6'(1'H,3'H)-trione, 1,2,4,4a-tetrahydro-9-(4-methoxyphenyl)-2,4-dimethyl-, (2R,4S,4aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN

(Continued)

RN 679840-89-2 CAPLUS CN Spiro[(1,4) oxarino[4,3-a] quinoline-5(6H),5'(2'H)-pyrimidine]-2',4',6'(1'H,3'H)-trione, 9-(3-chloco-4-fluorophenyl)-1,2,4,4a-tetrahydro-2,4-dimethyl-, (2R,4S,4aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

679840-90-5 CAPLUS
Spiro([1,4]0xazino(4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]2',4',6'(1'H,3'H)-trione, 1,2,4,4a-tetrahydro-2,4-dimethyl-9-(3-nitrophenyl)-, (2R,4S,4aS)- (9CI) (CA INDEX NAME)

L4 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

679840-91-6 CAPLUS Benzonitrile, 4-[(2R,4S,4aS)-1,1',2,3',4,4',4a,6'-octahydro-2,4-dimethyl-

2',4',6'-trioxospiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidin]-9-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

679840-92-7 CAPLUS
Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'[2'H)-pyrimidine]2',4',6'['H,3'H)-trione, i,2,4,4a-tetrahydro-2,4-dimethyl-9-[4-(methylsulfonyl)phenyl]-, (2R,4S,4aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 2 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

679840-95-0 CAPLUS
Benzoic acid, 3-[(2R,4S,4aS)-1,1',2,3',4,4',4a,6'-octahydro-2,4-dimethyl-

2',4',6'-trioxospiro[(1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidin}-9-yl]-, methyl ester {9CI) (CA INDEX NAME)

Absolute stereochemistry.

581006-33-7 CAPLUS
Spiro[[1,4]0xazino[4,3-a]quinoline-5[6H],5'(2'H)-pyrimidine]2',4',6'(1'H,3'H)-trione, 1,2,4,4a-tetrahydro-2,4-dimethyl-8-nitro-,
(2R,4S,4aS)-[9CI] (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

RN 679840-93-8 CAPLUS
CN Spiro[[1,4]oxazino[4,3-a]quinoline-5[6H],5'(2'H)-pyrimidine]2',4',6'(1'H,3'H)-trione,
1,2,4,4a-tetrahydro-2,4-dimethyl-9-(4-pyridinyl), (2R,4S,4aS)- (9CI) (CA INDEX NAME)

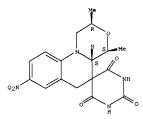
Absolute stereochemistry.

679840-94-9 CAPLUS Benzoic acid, 4-{(2R,45,4a5)-1,1',2,3',4,4',4a,6'-octahydro-2,4-dimethyl-

2',4',6'-trioxospiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidin]-9-yl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



REFERENCE COUNT:

THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

L4 ANSWER 3 OF 11 CAPLUS COPYRIGHT 2004 ACS ON STN ACCESSION NUMBER: 2004:43955 CAPLUS 140:286965

DOCUME TITLE: 140:286965
Thermochemical study on the ring closure reaction of 5-morpholino-4-vinylpyridazinones by tert-amino

effect AUTHOR(S): Beke, Karolyhazy, Laszlo; Regdon, Geza; Elias, Oliver; Gyula; Tabi, Tamas; Hodi, Klara; Eros, Istvan;

Matyus, Peter

CORPORATE SOURCE:

Peter Department of Organic Chemistry, Semmelweis University, Budapest, 1992, Hung. THEOCHEM (2003), 666-667, 667-668 CODEN: THEODJ: ISSN: 0166-1280 Elsevier Science B.V. SOURCE: PUBLISHER .

DOCUMENT TYPE: LANGUAGE: AB Cyclizatio

MENT TYPE: Journal
UAGE: English
Cyclization of tert-anilines with a properly substituted vinyl moiety by
the tert-amino effect affords fused pyridines. This type of ring closure
reaction of 5-morpholino-4-vinylpyridazinones and a benzene analog was
investigated by differential scanning calorimetry (DSC) measurements.

methods. The enthalpy values and heats of reactions were obtained from the thermograms by integrating the peak area corresponding to the ring-closure reaction, and by semiempirical (PM3) and DFT (d. function theory) calcns., resp. 675597-19-09
Ri: RPR (Properties); SPN (Synthetic preparation); PREP (Preparation) (melting temperature; DSC and PM3 and DFT study on the thermochem. of

closure reaction of 5-morpholino-4-vinylpyridarinones induced by
 tert-amino effect)
675597-19-0 CAPLUS
Spiro[[1,4]oxazino[4,3-a]quinoline-5(6H),5'(2'H)-pyrimidine]2',4',6'(1'H,3'H)-trione, 1,2,4,4a-tetrahydro-1',3'-dimethyl- (9CI) (CA
TUNEY NUMB.)

REFERENCE COUNT:

10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR

RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

ACCESSION NUMBER:

DOCUMENT NUMBER:

ANSWER 4 OF 11 CAPLUS COPYRIGHT 2004 ACS ON STN

SSION NUMBER: 1999:468342 CAPLUS

131:102292
E: 131:102292
acridinone derivatives and their nitrogen-containing tri- and tetracyclic analogs as antiviral agents Furta, Yosuke; Sugita, Atsushi: Uehara, Sayuri; Takahashi, Kazumi; Nagaki, Hideyoshi; Kamina, TITLE: INVENTOR(S):

Hiroshi;

Shiraki, Kimiyasu Toyama Chemical Co., Ltd., Japan Jpn. Kokai Tokkyo Koho, 74 pp. CODEN: JKXXAF PATENT ASSIGNEE(S): SOURCE:

DOCUMENT TYPE: Patent Japanese

LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 11199565 PRIORITY APPLN. INFO.:	A2	19990727	JP 1998-294339 JP 1997-303545	19981016 19971017

OTHER SOURCE(S): MARPAT 131:102292

The title compds. [I; Rl = {un}substituted alkyl, alkenyl, cycloalkyl, aryl, or heterocyclyl; R2 = {un}substituted aryl or heterocyclyl; R3 = H, halo, {un}protected OH, NH2, or CO2H, {un}substituted alkyl; R4 = H,

halo, (un)protected OH, NHZ, OF COZH, (un)substituted stays, NA - NA, halo;

Al, A2 = N, CH; A3 = CH or A3 and R1 together form optionally alkyl-substituted CH2CH2-B; B = 0, NH] are prepared They are useful as antiviral agents, in particular anti-herpes simplex virus (anti-HSV) agents. Thus, (10-bromo-5-fluoro-7-cxo-1,2-dihydro-7H-[1,4]oxazino[2,3,4-de]acridin-2-yl)methyl accetate was coupled with 2-(1,1)-trimethylstannyl) - 1,3-thiazole in the presence of bis(triphenylphosphine)palladium dichloride in xylehe under reflux, followed by saponification to give 5-fluoro-2-(hydroxymethyl)-10-[1,3-thiazol-2-yl)-1,2-dihydro-7H-[1,4]oxazino[2,3,4-de]acridin-7-one (II). Il in vitro inhibited HSV-2 with ICSO of 0.08 µg/mL. Pharmaceutical formulations containing I were also prepared wich (CDU of 0.08 µg/mL. Pharmaceutical formulations containing also prepared

IT 231625-08-4P 231625-10-8P 231625-11-9P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological)

ogical study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of heterocyclyldihydroacridinone derivs. and their

BIOL

L4 ANSWER 4 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
nitrogen-contg. tri- and tetracyclic analogs as antiviral agents)
RN 231625-08-4 CAPLUS
CN 7H-[1,4]Oxazino[2,3,4-de]acridin-7-one,
5-fluoro-1,2-dihydro-10-(1H-1,2,4triazol-1-y1)- (9CI) (CA INDEX NAME)

RN 231625-10-8 CAPLUS
CN 7H-[1,4]Oxazinc[2,3,4-de]acridin-7-one,
2-[(acetyloxy)methyl]-5-fluoro-1,2dihydro-10-[2-thiazolyl)- (9cI) (CA INDEX NAME)

231625-11-9 CAPLUS 7H-[1,4]Oxazino[2,3,4-de]acridin-7-one, 5-fluoro-1,2-dihydro-2-(hydroxymethyl)-10-(2-thiazolyl)- (9CI) (CA INDEX NAME)

231626-13-4

231626-13-4
RE: RCT (Reactant); RACT (Reactant or reagent)
{preparation of heterocyclyldihydroacridinone derivs. and their
nitrogen-containing tri- and tetracyclic analogs as antiviral agents)
231626-13-4 CAPUS
7H-[1,4]0xazino[2,3,4-de]acridin-7-one, 2-[(acetyloxy)methyl)-1-bromo-5fluoro-1,2-dihydro- (SCI) (CA INDEX NAME)

10/27/2004

Habte

L4 ANSWER 4 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

231625-90-4F 231625-98-2F 231625-99-3F
RE: RCT (Reactant); SPN (Synthetic preparation); PREF (Preparation); RACT (Reactant or reagent)
(preparation of heterocyclyldihydroacridinone derivs. and their nitrogen-containing tri- and tetracyclic analogs as antiviral agents)
231625-90-4 CAPLUS
7H-[1,4]0xazino[2,3,4-de]acridin-7-one, 5,10-difluoro-1,2-dihydro- (SCI)
(CA INDEX NAME)

231625-98-2 CAPLUS 7H-[1,4]OXazino[2,3,4-de]acridin-7-one, 10-bromo-5-fluoro-1,2-dihydro-(9CI) (CA INDEX NAME)

231625-99-3 CAPLUS 7H-[1,4]Oxazino[2,3,4-de]acridin-7-one, 2-[(acetyloxy)methyl]-10-bromo-5-flooro-1,2-dihydro- [9CI) (CA INDEX NAME)

ACCESSION NUMBER:

DOCUMENT NUMBER: TITLE:

ANSWER 5 OF 11 CAPLUS COPYRIGHT 2004 ACS ON STN
SSION NUMBER: 1995:711926 CAPLUS
MENT NUMBER: 123:285825
E: Synthesis of tricyclic cyano-substituted
tetrahydroquinolines by radical decyanation of

dinitriles
Gerlach, Uwe
Hoechst Ag, Frankfurt, 65296, Germany
Tetrahedron Letters (1995), 36(29), 5159-62
CODEN: TELEAY; ISSN: 0040-4039
Elsevier
Journal
English
CASREACT 123:285825

AUTHOR (S):

CORPORATE SOURCE:

SOURCE:

PUBLISHER: DOCUMENT TYPE:

LANGUAGE:

OTHER SOURCE(S):

geminal

Various dicyanides I (X = bond, CH2, NMe, O, S, SO, SO2) of tricyclic tetrahydroquinoline derivs. were converted to their monocyanides in high yield by reductive radical decyanation with tributyltin hydride and 2,2'-azobisisobutyronitrile (AIBN). 97699-07-8

169778-23-8P 169778-24-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(synthesis of tricyclic cyano-substituted tetrahydroquinolines by radical decyanation of geminal dinitriles)
169778-23-8 CAPLUS
(1,4) Oxazino (4,3-a) quinoline-5-carbonitrile, 1,2,4,4a,5,6-hexahydro-,trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.

Habte

L4 ANSWER 4 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN

(Continued)

ANSWER 5 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN

(Continued)

169778-24-9 CAPLUS [1,4] Oxazino[4,3-a] quinoline-5-carbonitrile, 1,2,4,4a,5,6-hexahydro-,

(9CI) (CA INDEX NAME)

10/677,551

Page 20

ACCESSION NUMBER: 1989:38857 CAPLUS DOCUMENT NUMBER: 110:38857 CAPLUS TITLE: Stereochemical aspects of the 2.

Stereochemical aspects of the "tert-amino effect".

Enantio- and diastereoselectivity in the synthesis of quinolines, pyrrolo[1,2-a]quinolines, and [1,4]oxazino[4,3-a]quinolines Nijhuis, Walter H. N.; Verboom, Willem; Abu El-Fadl, A.; Van Hummel, Gerrit J.; Reinhoudt, David N. Lab. Org. Chem., Univ. Twente, Enschede, 7500 AE, Neth. AUTHOR(S): CORPORATE SOURCE:

Neth. Journal of Organic Chemistry (1989), 54(1), 209-16 CODEN: JOCEAH, ISSN: 0022-3263 Journal

SOURCE:

DOCUMENT TYPE: LANGUAGE: OTHER SOURCE(S): GI

English CASREACT 110:38857

AB Thermal isomerization of the optically pure 2-vinyl-N,N-dialkylanilines, with a Me or an E substituent at the α -position of the N,N-dialkyl molety, affords enantioselectively the optically pure pyrrolo[1,2-a] equinolines and the [1,4] chazzino[4,3-a] equinoline, with the Me or Et substituent at the bridgehead C atom, and the quinoline, resp. The optical purity of these quinoline derivs. was determined by JH-MMR spectroscopy in the presence of chiral shift reagents. Heating of the optically pure analogs in which the substituent is a methoxymethyl group in refluxing 1-butanol yields, besides the compds. With the methoxymethyl group at the bridgehead carbon atom, also the regionsomers that are enantiomerically pure. Mixts. of the diastereomers e.g. I (R, Rl = H, Me) were obtained by

cyclization of compound e.g. II, with a 3-ethylmorpholinyl group, in refluxing 1-butanol. The compds, were proven enantiomerically pure. The configuration of the compds, were determined by x-ray anal. of I (R = H,

R1 = Me) and 1H-NMR, and 1H-NOE difference spectroscopy. These results provide conclusive evidence for the mechanism of these cyclization reactions, which are further examples of the "tert-amino effect". The effect of substituents on the enantio- and diastereoselectivity of the cyclization is discussed.

is discussed. IT 117607-21-3P 117607-28-0P

ANSWER 6 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

117607-22-4 CAPLUS [1,4]Oxazino[4,3-a]quinoline-5,5(6H)-dicarbonitrile, 4a-ethyl-1,2,4,4a-etrahydro-6-methyl-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.

1./5//-gy-1 CAPAUAS [1,4]Oxazino[4,3-a]quinoline-5,5(6H)-dicarbonitrile, 4a-ethyl-1,2,4,4a-tetrahydro-6-methyl-, (4as-trans)- (9CI) (CA INDEX NAME) 117677-89-1 CAPLUS

Absolute stereochemistry.

117677-90-4 CAPLUS
[1,4]Cxazino[4,3-a]quinoline-5,5(6H)-dicarbonitrile, 4a-ethyl-1,2,4,4a-tetrahydro-6-methyl-, (4aS-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Answer 6 of 11 caplus copyright 2004 ACS on STN (Continued)
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and crystal structure of)
117607-21-3 CAPLUS
[1,4] OXAZINO[4,3-a] quinoline-5,5(6H)-dicarbonitrile, 4a-ethyl-1,2,4,4a-tetrahydro-6-methyl-, trans- (SCI) (CA INDEX NAME)

Relative stereochemistry.

RN 117607-28-0 CAPLUS CN [1,4]Oxazino[4,3-a]quinoline-5,5(6H)-dicarbonitrile, 1,2,4,4a-tetrahydro-6-methyl-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.

117607-20-2P 117607-22-4P 117677-89-1P

117677-90-4P RL: SPN (Synthetic preparation); PREP (Preparation)

Absolute stereochemistry.

(preparation of)
117607-20-2 CAPLUS
(1,4]Oxazino[4,3-a]quinoline-5,5(6H)-dicarbonitrile, 4a-ethyl-1,2,4,4a-tetrahydro-, (S)- (9CI) (CA INDEX NAME)

ANSWER 6 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

18

L4 ANSWER 7 OF 11 CAPLUS COPYRIGHT 2004 ACS ON STN ACCESSION NUMBER: 1984:611257 CAPLUS DOCUMENT NUMBER: 101:211257

A novel method for heteroatom-substituted free TITLE: radical

AUTHOR (S):

generation by photochemical electron transfer induced desilylation of RKCH2SiMe3 systems Rrumfield, Martha A.; Quillen, Suzanne L.; Yoon, Ung Chan; Mariano, Patrick S. Dep. Chem., Univ. Maryland, College Fark, MD, 20742, USA

CORPORATE SOURCE:

USA Journal of the American Chemical Society (1984), 106(22), 6855-6 CODEN: JACSAT; ISSN: 0002-7863 Journal English

DOCUMENT TYPE:

SOURCE:

$$\bigcap_{\mathbf{H}}^{\mathbf{Ph}}_{\mathbf{CH}_{2}\mathsf{XR}} \quad \mathbf{I} \qquad \bigcap_{\mathbf{0}} \quad \mathbf{I}$$

AB Irradiation of 2-phenyl-1-pyrrolinium perchlorate in MeCN containing RXCH2SiMe3

(RX = EtO, Me2CHO, EtS) leads to generation of the corresponding adducts

(same RX), arising by pathways involving excitation, singlet state electron transfer, cation radical desilylation, and ultimate radical pair coupling. Similarly, intramol. processes proceeding through these routes lead to production of heterocyclic products. Thus, (trimethylsilylmethoxyalkyl)quinolinium salts produce cyclic ethers,

II, when irradiated in MeCN, followed by hydrogenation.
40971-38-0F
RE: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
40971-38-8 CAPLUS
[1,4]Oxazino[4,3-a]quinoline, 1,2,4,4a,5,6-hexahydro- (9CI) (CA INDEX NAME)

ACCESSION NUMBER:

DOCUMENT NUMBER:

TITLE:

ANSWER 8 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN

SSION NUMBER: 1984:51477 CAPLUS

100:51477

E: "Tert-Amino effect" in heterocyclic synthesis.

Formation of N heterocycles by ring-closure reactions of substituted 2-vinyl-N,N-dialkylanilines

OR(5): Verboom, Willem; Reinhoudt, David N.; Visser,

AUTHOR (S): Richard;

Harkema, Sybolt
Twente Univ. Technol., Enschede, 7500 AE, Neth.
Journal of Organic Chemistry (1984), 49(2), 269-76
CODEN: JOCEAH; ISSN: 0022-3263
Journal CORPORATE SOURCE: SOURCE:

DOCUMENT TYPE:

LANGUAGE: OTHER SOURCE(S): GI English CASREACT 100:51477

AB 2-Vinyl-N,N-dialkylanilines react thermally in polar solvents and/or in the presence of Lewis acids via [1,5] or [1,6] hydrogen transfer followed by C-C bond formation to give heterotricyclic compds. The reaction depends on the type of N,N-dialkylamino group and on the type and position of substituents of the vinyl moiety. Di-Me 1-pyrrolidinyl butenedioate and (1-pyrrolidinyl)benzeneacetonitrile undergo a thermal rearrangement to

the pyrrolo[1,2-a]indoles I (R = RI = CO2Me; R = cyano, RI = Ph), resp., while the 1-piperidinyl and 4-morpholinyl butenedioates and (4-morpholinyl) butenedioates and (4-morpholinyl) benzeneactonitrile do not react. (I = Piperidinyl) benzeneactonitrile do not react. (I = Piperidinyl) benzeneactonitrile vicids in refluxing PhMe in the presence of Zncl2 the pyrido[1,2-a]indole II and its HCN elimination product. Under these conditions cis- and trans-I (R = cyano, R1 = Ph) also eliminate HCN. Heating the III (R2 = CO2Me, cyano, X = bond; R2 = cyano, X = CH2, O) in BuOH gives pyrrolo[1,2-a]quinolines, benzo[c]quinolitrine and [1,4]oxazino[4,3-a]quinoline derivs., resp. The mechanisms of both types of cyclization, which are examples of the tert-amino effect, are discussed.

87689-07-BP
RI: SDN (Synthetic preparation); PREP (Preparation)

87699-07-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
87699-07-8 CAPLUS
[1,4]Oxazino[4,3-a]quinoline-5,5(6H)-dicarbonitrile, 1,2,4,4a-tetrahydro-(9CI) (CA INDEX NAME)

L4 ANSWER 7 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN

(Continued)

ANSWER 8 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN

(Continued)

L4 ANSWER 9 OF 11
ACCESSION NUMBER:
DOCUMENT NUMBER:
1980:146175 CAPLUS
92:146175 CAPLUS
92

LANGUAGE: German CASREACT 92:146175 OTHER SOURCE(S):

Heterocyclic derivs. (e.g., I; Y = PhCMe, CO, CS, CH2, NEt, O, S) or naphth $\{3,2,1-dc\}$ anthracenes, which can be represented by skeleton types

(X = methylene group, CO; Y = S, methylene or imino group, CS, CO, O, bond: Z = N, C+, C-) or III (X = methylene group, Y = C, Z = N+, C; R undefined), are helically distorted in the stereochem. ground state. 11

racemize so fast, however, that their free enthalpy of racemization (AG \leq 21 kcal/mol) can be determined by standard dynamic NMR methods Only type I compds. with relatively large bridges (Y = PhCMe or S) sit

higher racemization barriers. The latter had to be determined by

equilibrium methods. The results indicate that for II and III regement of bridges Y and/or X and diminution of Z should increase nonbonding interactions in the planar transition state and therefore increase the racemization barrier. For substituted I (Y = CMe2) derivs., IH NMR signals of diastereotropic and constitutopic groups were found to coincide.

73183-70-7P RE: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
73183-70-7 CAPLUS
9H-Quino[3,2,1-k1]phenoxazine, 9,9-dimethyl- (SCI) (CA INDEX NAME)

L4 ANSWER 10 OF 11 CAPLUS COPYRIGHT 2004 ACS ON STN
ACCESSION NUMBER: 1973:124521 CAPLUS
DOCUMENT NUMBER: 78:124521
TITLE: Synthesis of 1,2,4,4a,5,6-hexahydro-1,4-oxazino[3,4-a]quinolines
AUTHOR(5): Rao, V. Atuna; Jain, Padam C.; Anand, Nitya
CORPORATE SOURCE: COLEN: Inst., Lucknow, India
SOURCE: Indian Journal of Chemistry (1972), 10(12), 1134-5
CODEN: IOCAP; ISSN: 0019-5103
DOCUMENT TYPE: Dournal
LANGUAGE: English
GT For diagram(s), see printed CA Issue.
AB 1,2,4,4a,5,6-Hexahydro-1,4-oxazino[3,4-a]quinoline (I R = H) and its
2-methyl- and 2-phenyl derivs. have been synthesized starting from Me
1,2,3,4-tetrahydroquinaldate (II). II on biAliki reduction, followed by
treatment with ethylene oxide, gives 1-β-hydroxymethyl-1,2,3,4-tetrahydroquinoline (II, R = H). The latter on treatment with
48% HB: gives I (R = H). Condensation of 2-hydroxymethyl-1,2,3,4-tetrahydroquinoline with styrene and propylene oxides gives the
corresponding I is mixts. of diastereoisomers. The stereochem of the
substituents at 2-position has been proposed on the basis of NMR data.

IT 40971-38-87 40971-39-97 40971-42-4P
40971-38-87 40971-39-99 40971-42-4P
40971-38-87 40971-39-99 40971-42-4P
40971-38-88 CAPLUS
CN [1,4]Oxazino[4,3-a]quinoline, 1,2,4,4a,5,6-hexahydro- (9CI) (CA INDEX
NNME)

[1,4]Oxazino[4,3-a]quinoline, 1,2,4,4a,5,6-hexahydro- (9CI) (CA INDEX

40971-39-9 CAPLUS (1,4)Oxazino[4,3-a]quinolin-1(2H)-one, 4,4a,5,6-tetrahydro- (9CI) (CA INDEX NAME)

103/1-42-4 CAPBUS
[1,4]OXaZino[4,3-a]quinoline, 1,2,4,4a,5,6-hexahydro-2-phenyl-, trans-(9CI) (CA INDEX NAME)

Relative stereochemistry.

ANSWER 9 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

ANSWER 10 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

40971-43-5 CAPLUS
[],4]Oxazino[4,3-a]quinoline, 1,2,4,4a,5,6-hexahydro-2-methyl- (9CI) (CA INDEX NAME)

40971-44-6 CAPLUS [1,4]Oxazino[4,3-a]quinoline, 1,2,4,4a,5,6-hexahydro-2-phenyl-, cis-(9CI) (CA INDEX NAME)

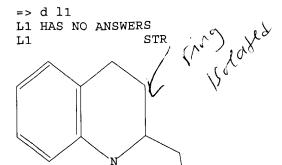
14 ANSWER 11 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN
1668:69015 CAPLUS
1668:69015 CAP

17591-45-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
17591-485-4 CAPLUS
9H-Quino(3,2,1-k1]phenoxazin-9-one (8CI) (CA INDEX NAME)

L4 ANSWER 11 OF 11 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

10/677,551

Page 3



Structure attributes must be viewed using STN Express query preparation.

=> s l1 SAMPLE SEARCH INITIATED 11:46:55 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 409 TO ITERATE

100.0% PROCESSED 409 ITERATIONS

2 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS:

6967 TO 9393

PROJECTED ANSWERS:

2 TO 124

L2

2 SEA SSS SAM L1

=> s l1 sss full FULL SEARCH INITIATED 11:47:04 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 7865 TO ITERATE

100.0% PROCESSED 7865 ITERATIONS

20 ANSWERS

SEARCH TIME: 00.00.01

T.3 20 SEA SSS FUL L1

=> file caplus
COST IN U.S. DOLLARS

SINCE FILE TOTAL

ENTRY SESSION 155.42 155.63

FULL ESTIMATED COST

FILE 'CAPLUS' ENTERED AT 11:47:09 ON 27 OCT 2004 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2004 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications. The CA Lexicon is the copyrighted intellectual property of the

10/27/2004

Habte

Page 4

American Chemical Society and is provided to assist you in searching databases on STN. Any dissemination, distribution, copying, or storing of this information, without the prior written consent of CAS, is strictly prohibited.

FILE COVERS 1907 - 27 Oct 2004 VOL 141 ISS 18 FILE LAST UPDATED: 26 Oct 2004 (20041026/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 13

10/677,551

L4 6 L3

=> d ibib abs hitstr tot





L4 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2004:308443 CAPLUS
DOCUMENT NUMBER: 140:339202
TITLE: Preparation of tricyclic tetrahydroquinoline antibacterial agents
INVENTOR(S): Barbachyn, Michel Robert; Dobrowolski, Paul Joseph; Hurd, Alexander Ross; McNamara, Dennis Joseph; John Raymond: Romero, Arthur Glenn; Ruble, James Craig; Sherry, Debra Ann; Thomasco, Lisa Marie; Toogood, Peter Laurence Pharmacia & Upjohn Company, USA PCT Int. Appl., 128 pp. CODEN: PIXXD2 Patent English 1 Palmer,

PATENT ASSIGNEE(S): SOURCE:

DOCUMENT TYPE:

LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

						KIND DATE			APPLICATION NO.						DATE		
	WO 2004031195				A1 20040415			WO 2003-IB4389									
#0	W-	DE	DG.	AT	.MA	AT.	AU,	AZ.	BA.	BB,	BG,	BR,	BY,	BZ,	CA,	CH,	CN,
		CO,	CB.	CU.	CZ.	DE.	DK,	DM.	DZ.	EC.	EE.	EG,	ES,	FI,	GB,	GD,	GE,
		GH,	GM.	HR.	HU.	TD.	IL,	IN.	IS.	JP,	KE.	KG,	KP,	KR,	KZ,	LC,	LK,
		T.D	1.5	LT	Tall.	LV.	MA,	MD.	MG.	MK.	MN.	MW,	MX,	MZ,	NI,	NO,	NZ,
		OM.	PG.	PH.	PL.	PT.	RO,	RU,	SC,	SD,	SE,	SG,	sĸ,	SL,	SY,	TJ,	TM,
		TN.	TR.	TT.	TZ.	UA.	UG,	US.	UZ,	VC,	VN,	YU,	ZA,	ZM,	ZW,	AM,	ΑZ,
				KZ,													
	RW:	GH.	GM.	KE.	LS.	MW.	MZ,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	ΑT,	BE,	ВG,
		CH.	CY.	CZ.	DE.	DK.	EE,	ES,	FI,	FR,	GB,	GR,	HU,	IE,	IT,	LU,	MC,
		NI.	PT.	RO.	SE.	SI,	SK,	TR,	BF,	ВJ,	CF,	CG,	CI,	CM,	GΑ,	GN,	GQ,
		GW.	MT	MR.	NE.	SN.	TD,	TG									
IIS	US 2004162279					,	2004	0819		US 2	003-	6775	51		2	0031	002
PRIORITY										US 2	002-	4166	85P		P 2	0021	007

US 2002-427189P P 20021118 US 2003-457622P P 20030326

OTHER SOURCE(S):

MARPAT 140:339202

ANSWER 1 OF 6 CAPLUS COPYRIGHT 2004 ACS on STN (Continued) [1,4]Oxazino[4,3-a]quinoline-5,5,8[6H)-tricarbonitrile, 1,2,4,4a-tetrahydro-2,4-dimethyl-, (2R,4S,4aR)-rel- (9CI) (CA INDEX

Relative stereochemistry

679839-65-7 CAPLUS [1,4]0xazino[4,3-a]quinoline-5,5(6H)-dicarbonitrile, 8-bromo-1,2,4,4a-tetrahydro-2,4-dimethyl-, (2K,4S,4aR)-rel- (9CI) (CA INDEX NAME)

679840-51-8 CAPLUS
[1,4]Oxazino[4,3-a]quinoline-5,5,8(6H)-tricarbonitrile,
1,2,4,4a-tetrahydro-2,4-dimethyl- (9CI) (CA INDEX NAME) CN

679840-52-9 CAPLUS [1,4]0xazino[4,3-a]quinoline-5,5(6H)-dicarbonitrile, 8-bromo-1,2,4,4a-tetrahydro-2,4-dimethyl- (9CI) (CA INDEX NAME)

ANSWER 1 OF 6 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

The invention includes tricyclic tetrahydroquinolines (shown as I; variables defined below; many of the examples are spiro compds., e.g.

and trans-II), and pharmaceutical compns. thereof, that exhibit useful antibacterial activity against a wide range of human and veterinary pathogens. For I: R1 is R12, C(O)R6, or CN; R2 = R12, C(O)R7, CN, CH2R7, NR17R7, CH2COR7, CH2CH2COR7; R3 = H, R2, O, C1-7 alkyl, C3-8 cycloalkyl, aryl, heteroaryl, or halo; each R4 = H, halo, OR12, OC(O)NR9R10, SR12, S(O)MR13, NR9R10, NR9S(O)MR13, NRSC(O)OR13, Ph, heteroaryl, cyano, nitro, CONR9R10, CO2R12, C(O)R13, C(:NOR12)R13, S(O)mMR9R10, NR9C(O)R12, C1-7 alkyl, C3-8 cycloalkyl, N3, hetl, or C(O)O-C1-4alkyl-R12; each R5 = H, C1-7alkyl, C3-8cycloalkyl, aryl or heteroaryl; x = -[C(R15)2]m-O-C(R15)2]m-NR16-[C(R15)2]k-, r20 is H, C1-7alkyl, C3-8cycloalkyl, aryl, or heteroaryl; Hetl is a C- or N-linked 5-8 membered mono- or bicyclic ring, each mono- or bicyclic ring being fully saturated or partially tdd.

тт

unsatd.,
and having 1-4 heteroatoms O, S, and N; hetl being (un)substituted by 1-2
substituents = cl-C4alkyl, amino, cl-C4alkylamino, cl-C4alkyloxy,

halogen, CN, O, or S; addnl. details including provisos are given in the claims.

method of preparation is claimed and .apprx.60 example prepns. are

used.
For example, cis- and trans-II were prepared in 3 steps starting with condensation of 2-fluoro-5-nitrobenzaldehyde with 2,6-dimethylmorpholine

condensation of 2-fluoro-5-nitrobenzaidenyde with 2,6-dimethylmotpholine to give cis- and trans-2-(2,6-dimethylmorpholin-4-yl)-5-nitrobenzaidehyde, each of which was condensed with barbituric acid to give cis- and trans-5-[2-(2,6-dimethylmorpholin-4-yl)-5-nitrobenzylidenelpyrimidine-2,4,6(1H,3H,5H)-trione, resp., each of which was cyclized in refluxing MeOH. Inhibition of E. coli DNR gyrase by 12 examples of I are reported.

IT 67840-52-9P 679840-62-5F 679840-81-6P 679840-51-0P 679840-51-0P GPS40-64-6F 079840-61-0P (Preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (USES)

(uses) (drug candidate; preparation of tricyclic tetrahydroquinoline antibacterial $% \left(\frac{1}{2}\right) =\frac{1}{2}\left(\frac{1}{2}\right) +\frac{1}{2}\left(\frac{1$

agents) 679839-64-6 CAPLUS

ANSWER 1 OF 6 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

679840-82-5 CAPLUS [1,4] Oxazino[4,3-a] quinoline-5,5,8(6H)-tricarbonitrile, 1,2,4,4a-tetrahydro-2,4-dimethyl-, (2R,45,4aS)- (9CI) (CA INDEX NAME)

679840-83-6 CAPLUS [1,4]Oxazino(4,3-a)quinoline-5,5(6H)-dicarbonitrile, 8-bromo-1,2,4,4a-tetrahydro-2,4-dimethyl-, (2R,4S,4aS)- (SCI) (CA INDEX NAME)

Absolute stereochemistry.

REFERENCE COUNT:

THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

10/677,551

Page 6

L4 ANSWER 2 OF 6 CAPLUS COPYRIGHT 2004 ACS ON STN
ACCESSION NUMBER: 1995:711926 CAPLUS
DOCUMENT NUMBER: 123:285825
Synthesis of tricyclic cyano-substituted
tetrahydroquinolines by radical decyanation of

dinitriles
Gerlach, Uwe
Hoechst AG, Frankfurt, 65296, Germany
Tetrahedron Letters (1995), 36(29), 5159-62
CODEN: TELEAY; ISSN: 0040-4039
Elsevier
Journal
English
CASREACT 123:285825 AUTHOR(S): CORPORATE SOURCE: SOURCE:

PUBLISHER: DOCUMENT TYPE: LANGUAGE: OTHER SOURCE(S):

Various dicyanides I (X = bond, CH2, NMe, O, S, SO, SO2) of tricyclic tetrahydroquinoline derivs. were converted to their monocyanides in high yield by reductive radical decyanation with tributyltin hydride and 2,2'-azobisisobutyronitrile (AIRN).
87699-07-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(synthesis of tricyclic cyano-substituted tetrahydroquinolines by radical decyanation of geminal dinitriles)
87699-07-8 CAPLUS
[1,4]Oxazino[4,3-a]quinoline-5,5(6H)-dicarbonitrile, 1,2,4,4a-tetrahydro-(9CI) (CA INDEX NAME) AB

IT

IT

169778-23-0P 169778-24-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(synthesis of tricyclic cyano-substituted tetrahydroquinolines by radical decyanation of geminal dinitriles)
169778-23-8 CAPLUS

ANSWER 2 OF 6 CAPLUS COPYRIGHT 2004 ACS on STN (Continued) [1,4]Oxazino[4,3-a]quinoline-5-carbonitrile, 1,2,4,4a,5,6-hexahydro-,trans- (9CI) (CA INDEX NAME)

169778-24-9 CAPLUS [1,4] Oxazino[4,3-a] quinoline-5-carbonitrile, 1,2,4,4a,5,6-hexahydro-,

(9CI) (CA INDEX NAME)

Relative stereochemistry.

L4 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2004 ACS ON STN ACCESSION NUMBER: 1989:38857 CAPLUS 10:38857

TITLE:

Stereochemical aspects of the "tert-amino effect".

AUTHOR(S): CORPORATE SOURCE: Enantio— and diastereoselectivity in the synthesis of quinolines, pyrrolo[1,2-a]quinolines, and [1,4]oxazino[4,3-a]quinolines and [1,4]oxazino[4,3-a]quinolines Nijhuis, Walter H. N.; Verboom, Willem; Abu El-Fadl, A.; Van Hummel, Gerrit J.; Reinhoudt, David N. Lab. Org. Chem., Univ. Twente, Enschede, 7500 AE, Neth. Journal of Organic Chemistry (1989), 54(1), 209-16 CODEN: JOCEAH; ISSN: 0022-3263 Journal

SOURCE:

DOCUMENT TYPE: LANGUAGE: OTHER SOURCE(S): GI English CASREACT 110:38857

Thermal isomerization of the optically pure 2-vinyl-N,N-dialkylanilines, with a Me or an E substituent at the α -position of the N,N-dialkyl moiety, affords enantioselectively the optically pure pyrrolo[1,2-alquinolines and the [1,4]oxazino[4,3-alquinoline, with the Me or Et substituent at the bridgehead C atom, and the quinoline, resp. The optical purity of these quinoline derivs. Was determined by IM-NMR troscopy

spectroscopy
in the presence of chiral shift reagents. Heating of the optically pure
analogs in which the substituent is a methoxymethyl group in refluxing
1-butanol yields, besides the compds. with the methoxymethyl group at the
bridgehead carbon atom, also the regioisomers that are enantiomerically
pure. Mixts. of the diastereomers e.g. I (R, Rl = H, Me) were obtained

cyclization of compound e.g. II, with a 3-ethylmorpholinyl group, in refluxing 1-butanol. The compds, were proven enantiomerically pure. The configuration of the compds, were determined by x-ray anal. of I (R = H,

Me) and 1H-NMR, and 1H-NOE difference spectroscopy. These results provide

ride conclusive evidence for the mechanism of these cyclization reactions, which are further examples of the "tert-amino effect". The effect of substituents on the enantio- and diastereoselectivity of the cyclization is discussed.

117607-21-3P 117607-28-0P
RL: PRP (Properties): SPN (Synthetic preparation); PREP (Preparation) (preparation and crystal structure of)
117607-21-3 CAPLUS
[1,4]Oxazino[4,3-a]quinoline-5,5[6H]-dicarbonitrile, 4a-ethyl-1,2,4,4a-

Habte

ANSWER 3 OF 6 CAPLUS COPYRIGHT 2004 ACS on STN tetrahydro-6-methyl-, trans- (9CI) (CA INDEX NAME) (Continued)

Relative stereochemistry.

RN 117607-28-0 CAPLUS CN (1,4)0xazino(4,3-a)quinoline-5,5(6H)-dicarbonitrile, 1,2,4,4a-tetrahydro-6-methyl-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry

IT

117607-20-2P 117607-22-4P 117677-89-1P
117677-90-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
117607-20-2 CAPLUS
[1,4]Oxazino(4,3-a]quinoline-5,5(6H)-dicarbonitrile, 4a-ethyl-1,2,4,4a-tetrahydro-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry

11/00/-22-4 CMFNDS [1,4]Oxazino[4,3-a]quinoline-5,5(6H)-dicarbonitrile, 4a-ethyl-1,2,4,4a-tetrahydro-6-methyl-, cis- (9CI) (CA INDEX NAME)

10/27/2004

10/677,551

Page 7

L4 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2004 ACS on STN (Continued) Relative stereochemistry.

117677-89-1 CAPLUS 11,4]Oxazino[4,3-a]quinoline-5,5[6H]-dicarbonitrile, 4a-ethyl-1,2,4,4a-tetrahydro-6-methyl-, (4as-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

117677-90-4 CAPLUS [1,4]0xazino[4,3-a]quinoline-5,5(6H)-dicarbonitrile, 4a-ethyl-1,2,4,4a-tetrahydro-6-methyl-, (4aS-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

1.4 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2004 ACS on STN

L4 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2004 ACS ON STN ACCESSION NUMBER: 1984:611257 CAPLUS COPURINT NUMBER: 101:211257 CAPLUS A novel method for heteroatom radical A novel method for heteroatom-substituted free generation by photochemical electron transfer induced desilylation of RXCHZSiMe3 systems
Brumfield, Martha A.; Quillen, Suranne L.; Yoon, Ung Chan; Mariano, Patrick S.
Dep. Chem., Univ. Maryland, College Park, MD, 20742, USA AUTHOR (S): CORPORATE SOURCE: USA Journal of the American Chemical Society (1984), 106(22), 6855-6 CODEN: JACSAT; ISSN: 0002-7863 Journal DOCUMENT TYPE: LANGUAGE: GI

AB Irradiation of 2-phenyl-1-pyrrolinium perchlorate in MeCN containing RXCH2SiMe3 (RX = EtO, Me2CHO, EtS) leads to generation of the corresponding adducts

(same RX), arising by pathways involving excitation, singlet state electron transfer, cation radical desilylation, and ultimate radical pair coupling. Similarly, intramol. processes proceeding through these routes lead to production of heterocyclic products. Thus, (trimethylsilylmethoxyalkyl)quinolinium salts produce cyclic ethers,

e.g., II, when irradiated in MeCN, followed by hydrogenation.
40971-38-8P
RI: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
40971-38-8 - CAPLUS
[1,4]0xazino[4,3-a]quinoline, 1,2,4,4a,5,6-hexahydro- (9CI) (CA INDEX IT

L4 ANSWER 5 OF 6 CAPLUS COPYRIGHT 2004 ACS on STN ACCESSION NUMBER: 1984:51477 CAPLUS

DOCUMENT NUMBER:

100:51477

100:51477
"Tert-Amino effect" in heterocyclic synthesis.
Formation of N heterocycles by ring-closure reactions
of substituted 2-vinyl-N,N-dialkylantlines
Verboom, Willem; Reinhoudt, David N.; Visser,

AUTHOR(S): Richard;

CORPORATE SOURCE:

Harkema, Sybolt Twente Univ. Technol., Enschede, 7500 AE, Neth. Journal of Organic Chemistry (1984), 49(2), 269-76 CODEN: JOCEAH; ISSN: 0022-3263 Journal

DOCUMENT TYPE: LANGUAGE:

English CASREACT 100:51477 OTHER SOURCE(S):

2-vinyl-N,N-dialkylanilines react thermally in polar solvents and/or in the presence of Lewis acids via [1,5] or [1,6] hydrogen transfer followed by C-C bond formation to give heterotricyclic compds. The reaction depends on the type of N,N-dialkylamino group and on the type and

position of substituents of the vinyl moiety. Di-Me 1-pyrrolidinyl butenedicate and (1-pyrrolidinyl)benzeneacetonitrile undergo a thermal rearrangement

and (1-pyrrolidinyl)benzeneacetonitrile undergo a thermal rearrangement the pyrrolo[1,2-a]indoles I (R = R1 = CO2Me; R = cyano, R1 = Ph), resp., while the 1-piperidinyl and 4-morpholinyl butenedioates and (4-morpholinyl)benzeneacetonitrile do not react. (1-Piperidinyl)benzeneacetonitrile yields in refluxing PhMe in the presence of Zncl2 the pyridol(1,2-a]indole II and its HCN elimination product. Under these conditions cis- and trans-I (R = cyano, R1 = Ph) also cellminate HCN. Heating the III (R2 = CO2Me, cyano, X = bond; R2 = cyano, X = CH2, O) in BuOH gives pyrrolo[1,2-a]quinolines, benzo[c]quinolizine, and [1,4]oxazino[4,3-a]quinoline derivs., resp. The mechanisms of both types of cyclization, which are examples of the tert-amino effect, are discussed.

87699-07-08
RL: SPN (synthetic preparation); PREP (Preparation)
(preparation of) 87699-07-08 CAPLUS
[1,4]Oxazino(4,3-a]quinoline-5,5(6H)-dicarbonitrile, 1,2,4,4a-tetrahydro-(SCI) (CA INDEX NAME)

L4 ANSWER 5 OF 6 CAPLUS COPYRIGHT 2004 ACS on STN

L4 ANSWER 6 OF 6 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1973:124521 CAPLUS
DOCUMENT NUMBER: 78:124521
TITLE: Synthesis of 1, 2, 4, 4a, 5, 6-hexahydro-1, 4-oxazino[3, 4-a]quinolines
AUTHOR(S): Rao, V. Aruna; Jain, Padam C.; Anand, Nitya
CORPORATE SOURCE: Cent. Drug Res. Inst., Lucknow, India
SOURCE: Indian Journal of Chemistry (1972), 10(12), 1134-5
CODEN: IJOCAP; ISSN: 0019-5103

DOCUMENT TYFE: Journal
LANGUAGE: English
GI Por diagram(s), see printed CA Issue.
AB 1,2,4,4a,5,6-Hexahydro-1,4-oxazino[3,4-a]quinoline (I R = H) and its
2-methyl- and 2-phenyl derivs. have been synthesized starting from Me
1,2,3,4-tetrahydroquinaldate (II). If on LiALH4 reduction, followed by
treatment with ethylene oxide, gives 1-β-hydroxymethyl-2-hydroxymethyl1,2,3,4-tetrahydroquinoline (II, R = H). The latter on treatment with
48% HBr gives I (R = H). Condensation of 2-hydroxymethyl-1,2,3,4tetrahydroquinoline with styrene and propylene oxides gives the
corresponding II (R = Ph, Me), which react with 48% HBr to give the
corresponding II (R = Ph, Me), which react with 48% HBr to give the
corresponding II (R = Ph, Me), which react with 48% HBr to give the
corresponding I as mixts. of diastereoisomers. The stereochem of the
substituents at 2-position has been proposed on the basis of NMR data.

17 40971-38-80971-43-9P 40971-42-4P
A0971-43-5F 40971-43-5P (A0971-43-5P 40971-43-5P (A0971-43-5P 40971-43-5P 40971-43-5P 40971-43-5P (A0971-43-5P 40971-43-5P 4097

40971-39-9 CAPLUS [1,4]Oxazino[4,3-a]quinolin-1(2H)-one, 4,4a,5,6-tetrahydro- (9CI) (CA INDEX NAME)

40971-42-4 CAPLUS [1,4]Oxazino(4,3-a]quinoline, 1,2,4,4a,5,6-hexahydro-2-phenyl-, trans-(9CI) (CA INDEX NAME)

L4 ANSWER 6 OF 6 CAPLUS COPYRIGHT 2004 ACS on STN Relative stereochemistry. (Continued)



40971-43-5 CAPLUS
[1,4]Oxazino[4,3-a]quinoline, 1,2,4,4a,5,6-hexahydro-2-methyl- (9CI) (CA INDEX NAME)



RN 40971-44-6 CAPLUS CN [1,4]Oxazino[4,3-a]quinoline, 1,2,4,4a,5,6-hexahydro-2-phenyl-, cis-(9CI) (CA INDEX NAME)